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FASCODE COMPUTER PROGRAM PREDICTIONS OF TYPICAL NO2 STACK PLUME--ETC(U)

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FASCODE COMPUTER PROGRAM PREDICTIONS OF TYPICAL NO_2 STACK PLUME SPECTRAL RADIATIVE PROPERTIES AS VIEWED FROM SPACE

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The FASCODE computer program has been exercised to determine the spectrum of a given NO_2 stack plume in the ($\nu_1 + \nu_3$) intercombination band at 3.4 μm as viewed from a space platform. The signal-to-background has been characterized both for the atmospheric radiance alone and for a black body earth as background and for the sum of both. Some comments are added concerning the reliability of the prediction and possible future work.

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LIST OF FIGURES

[redacted]

In this report we present results of an exercise of the FASCODE[1] computer program. We have used this code to try to determine the radiative properties of a particular assumed stack plume in the 3.4 μm region (2820, 2940 cm^{-1}). The plume has been taken to be twenty meters thick at or near the ground with a temperature of 296 K and an NO_2 concentration of one part per million. Note that ambient NO_2 concentrations near the ground are usually assumed to have a one part per billion mixing ratio[2]. We have in this first calculation, however, ignored ambient NO_2. This plume is viewed from a space platform looking vertically through the atmosphere. The absorber amount in the plume along this path is 5.094×10^{16} NO_2 molecules per cm^2, assuming that the U.S. Standard 1962 Atmosphere[3] gives the ambient total number density. Figure 1 shows the prediction of FASCODE for the radiance of the plume as a function of wave number. For comparison with possible instrumentation, the resolution of the line-by-line calculation has been degraded to 0.1 cm^{-1} using a rectangular convolution routine developed by L. Rothman at AFGL[4]. The line data for the calculation were taken from the AFGL trace gas line compilation[5]. The ordinate in Figure 1 is the log of the spectral radiance in watts cm^{-2} $ster^{-1}/(cm^{-1})$.

Figure 2 shows the transmission through the 1962 U.S. Standard Atmosphere over the same path for the same spectral region. Figure 3 gives the spectral radiance of this atmosphere in watts cm^{-2} $ster^{-1}/(cm^{-1})$ with no earthshine background. In Figure 4 we present the same calculation except for the addition of the plume as the lowest layer.

Increased emission can be noted at various points in the spectrum (e.g., at ~ 28[illegible], ~ 2890, ~ 2912, and ~ 2924 cm^{-1}). However, to demonstrate more clearly the relationship between these two spectra, the logarithm of one minus the ratio of the atmospheric radiance alone (Figure 3) to the sum of the atmospheric radiance and the plume (Figure 4) is plotted in Figure 5. This is the logarithm of the plume signal-to-background ratio where the background is the atmospheric emission neglecting earthshine. Comparing Figure 5 with Figure 1, one may readily see the rough outline of the plume radiance in Figure 5. Since the background atmospheric radiance itself is not very smooth (See Figure 3 for reference.) the signal-to-background ratio in Figure 5 reflects the background spectrum more strongly than it would were the background less strongly structured spectrally.

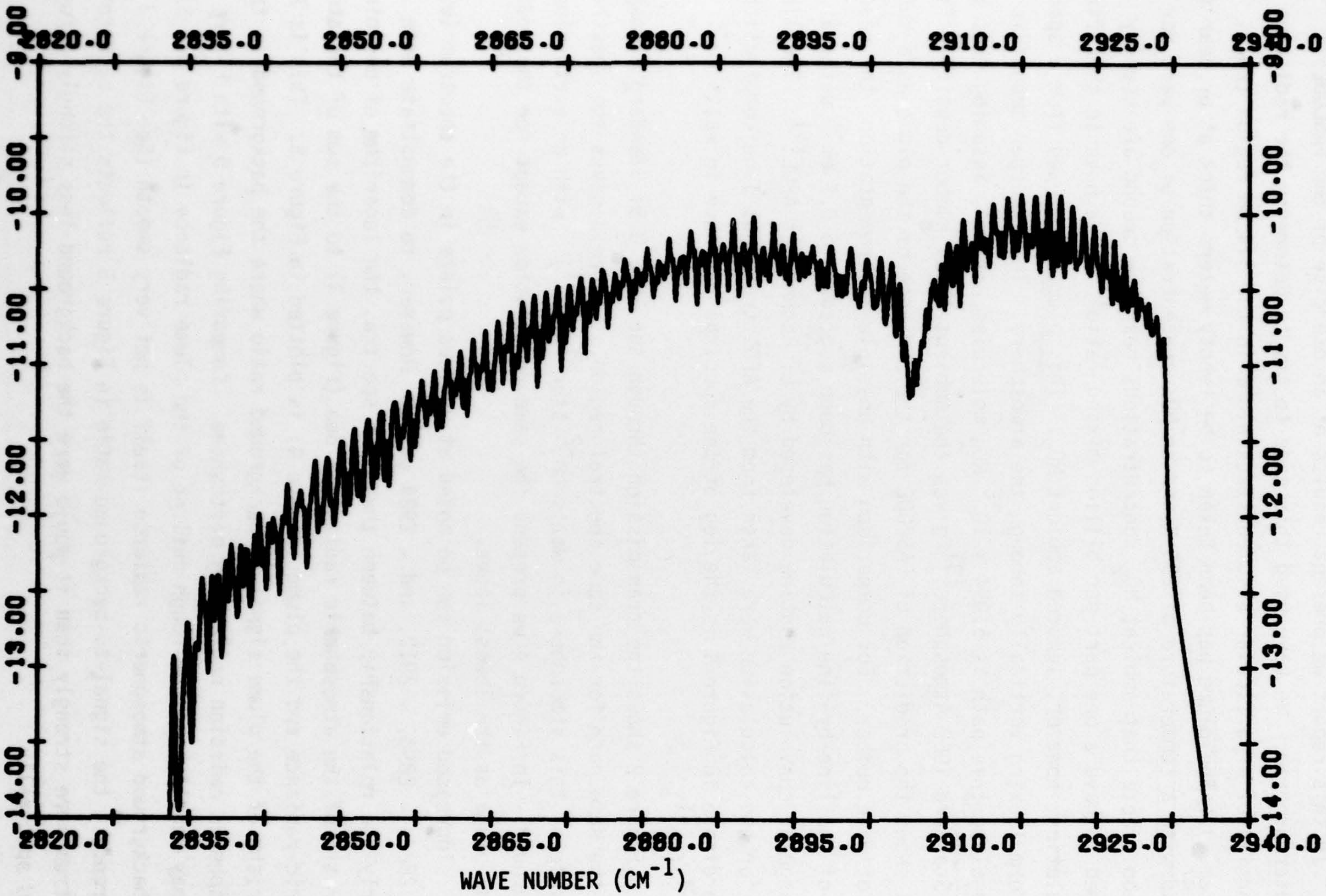

FIGURE 1: Logarithm of the Plume Spectral Radiance Only (watts/cm^2/ster/cm^{-1}).

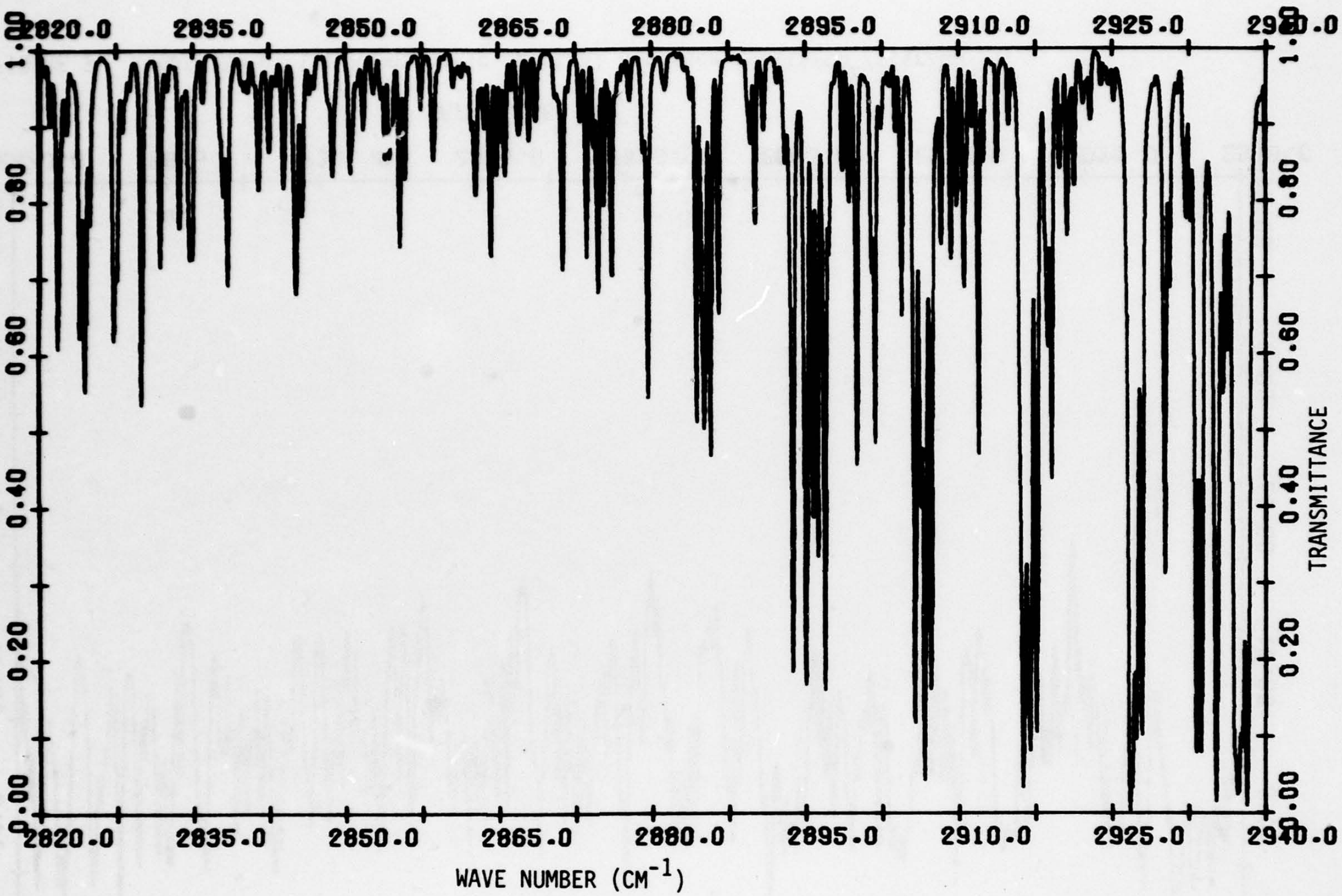

FIGURE 2: Atmospheric Transmittance as Viewed from Space Along a Vertical Path.

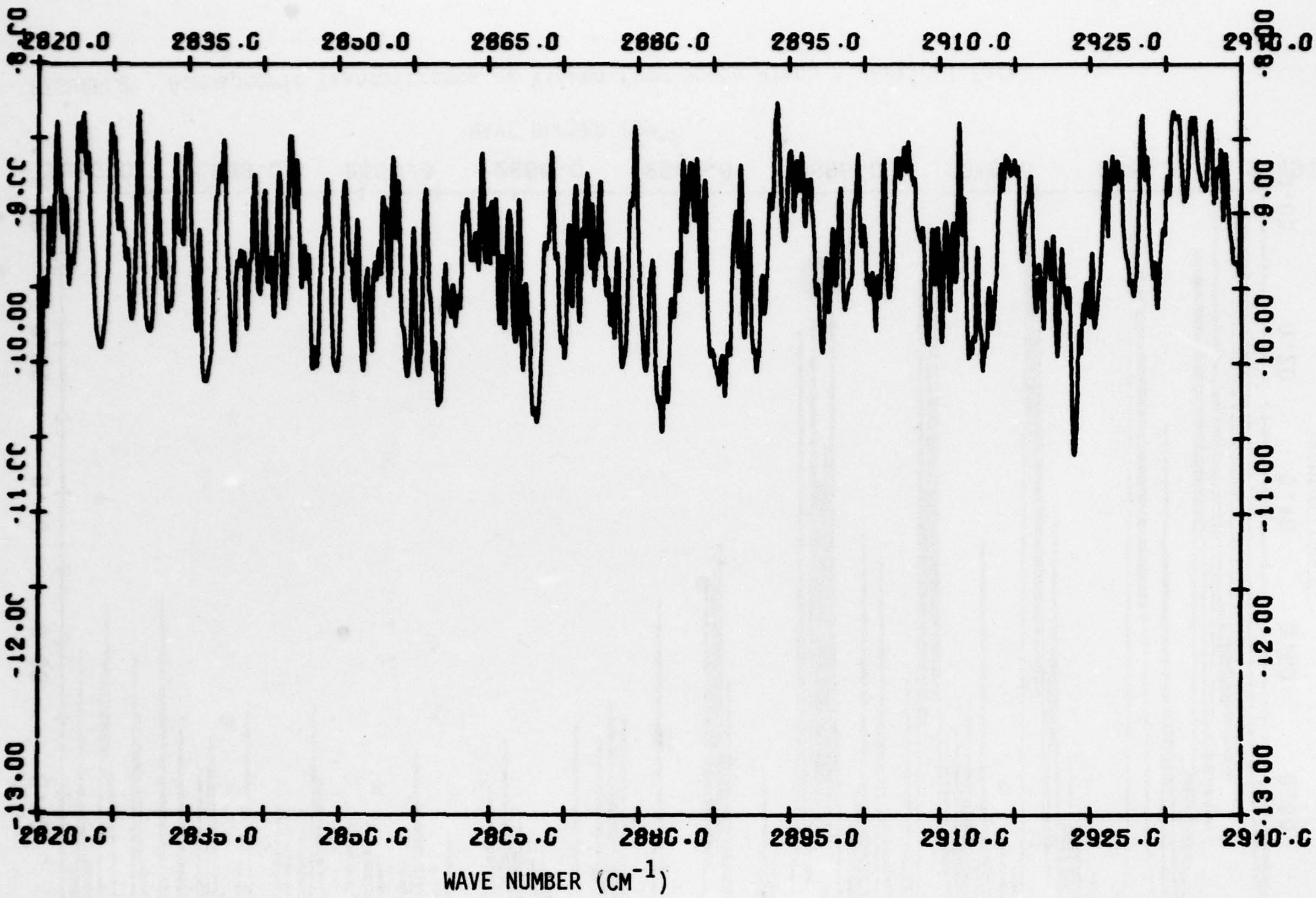

FIGURE 3: Logarithm of the Atmospheric Spectral Radiance (watts/cm^2/ster/cm^{-1}).

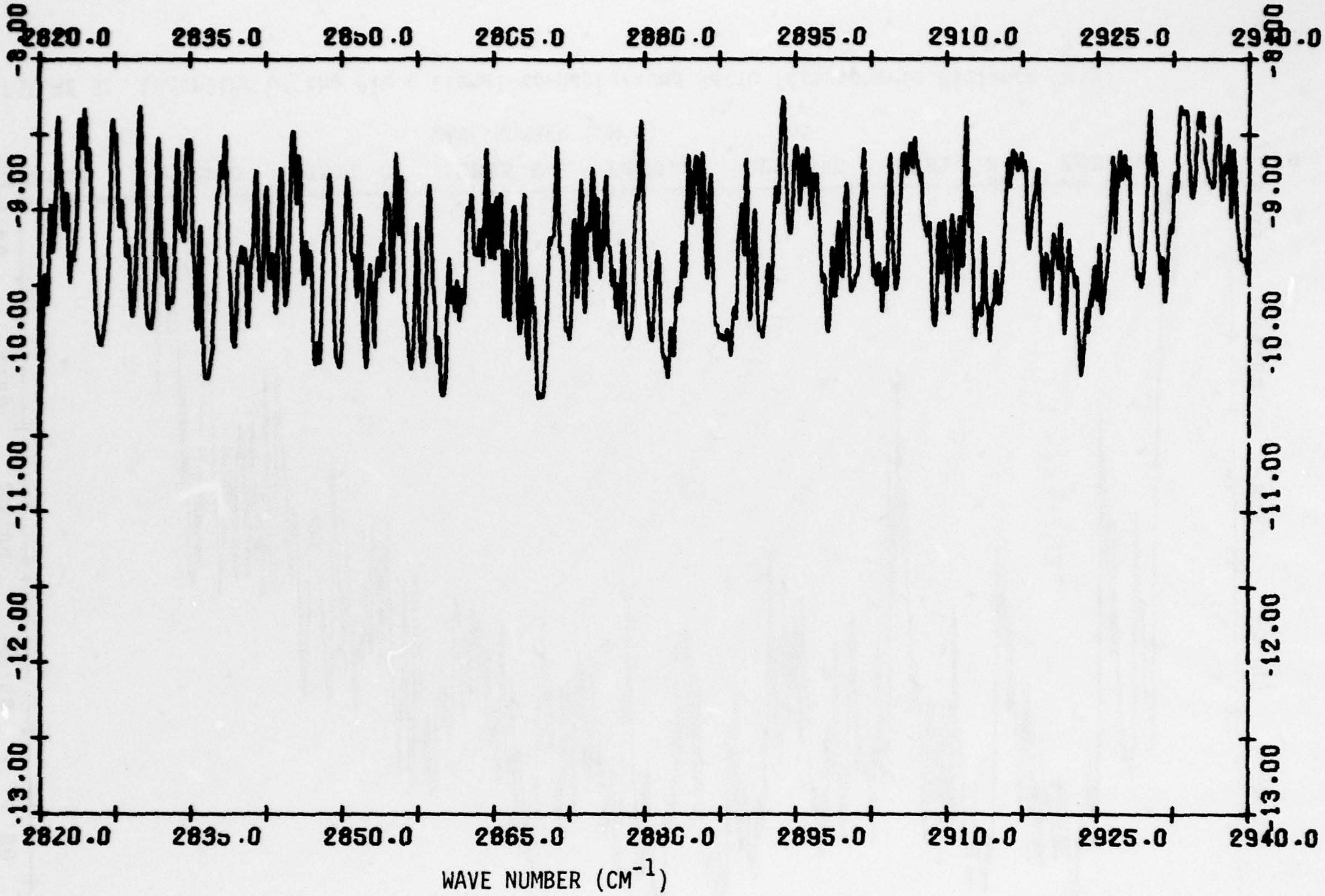

FIGURE 4: Logarithm of the Atmospheric Spectral Radiance (watts/cm^2/ster/cm^{-1}).

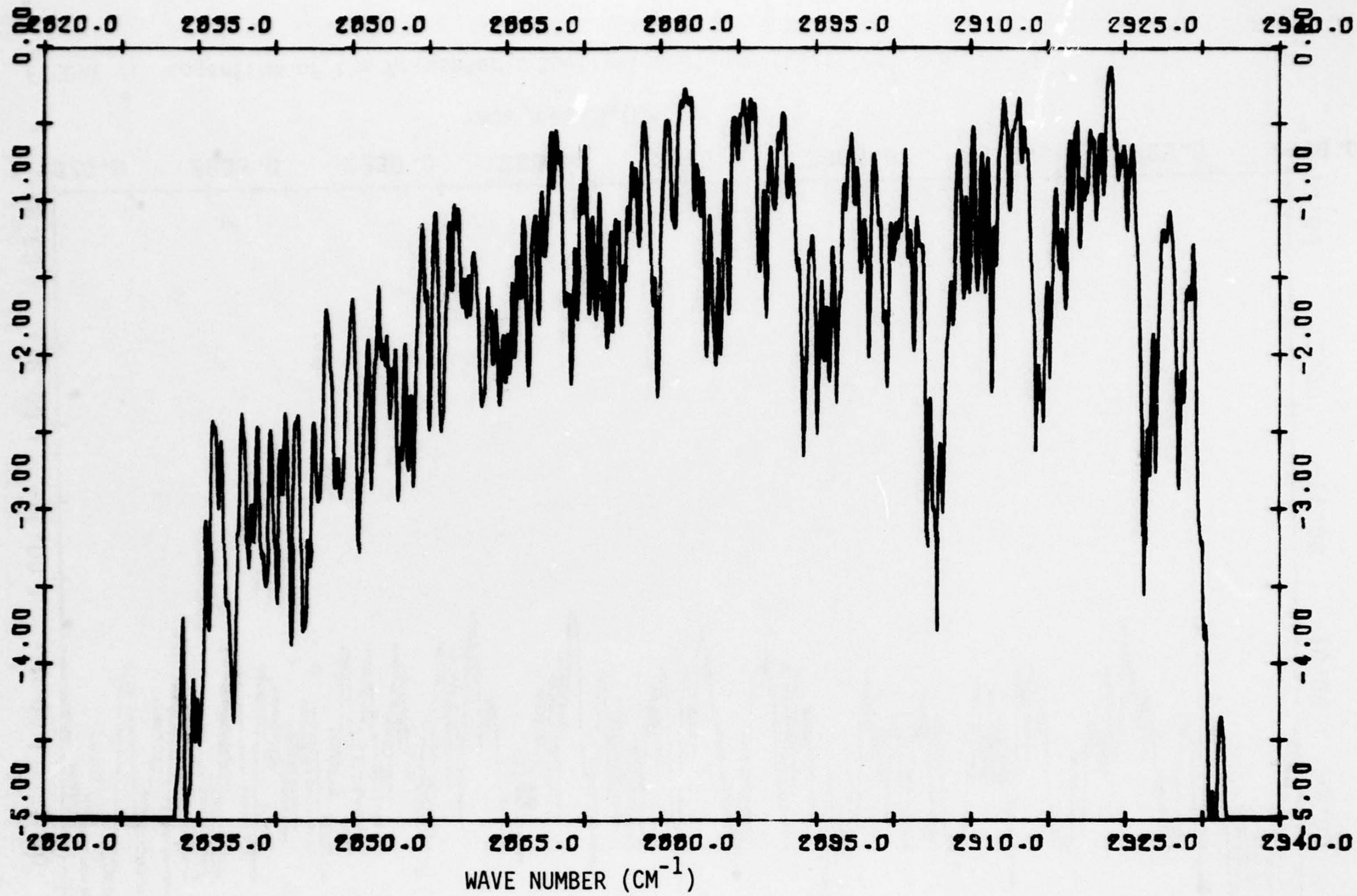

FIGURE 5: Logarithm of the Plume Signal-to-Background Ratio (Atmospheric Radiance Only).

In order to evaluate the effects of earthshine, the earth has been modelled as a black body radiating at 290 K, that is 6 K cooler than the plume. The spectral radiance as seen through the atmsophere for the case without the plume is shown in Figure 6 and for the case with the plume included, in Figure 7. *In Figure 8* we have plotted the logarithm of the ratio of the plume radiance seen through the atmosphere to the sum of the plume and the background. The general spectral shape of the plume radiance (Figure 1) is clearly seen with a few atmospheric absorption features modifying the output, e.g., near ~ 2915 and ~ 2925 cm^{-1}.

Comparing Figures 2 and 3, one sees the expected inverse relationship; namely that the atmosphere radiates most strongly in the spectral region where it is most strongly absorbing. The main difference that can be seen between Figures 3 and 4 is that the plume "fills in" some of the deeper notches in the equilibrium atmospheric radiance. Since these notches correspond to spectral regions where the transmission is nearly perfect, clearly one expects the additional radiance from the NO_2 plume to be more noticeable in the region of a notch.

The small difference between plume temperature and the black body temperature chosen to represent the earth background leads one to expect that the plume radiation would be difficult to detect against the background and indeed the naked eye can discern no differences between the spectra of Figures 6 and 7. However, the logarithmic ratio in Figure 8 shows the spectrum of $NO_2(\nu_1 + \nu_3)$ intercombination band quite faithfully except for a few absorption features due to the ambient atmosphere. Note that the background in this case is much less spectrally structured than that used in Figure 5. Thus the signal-to-background ratio reflects the plume spectrum more faithfully.

It is necessary at this point to point out the caveats. First, we note that the current FASCODE Program does not as yet treat a number of known phenomena such as the quasi-continua due to aerosol absorption and a variety of molecular processes. Also scattering has not been included. We argue that these omissions should not affect the above ratios greatly since the continuum effects will not change the plume signature greatly.

A more serious omission in the present study is the lack of ambient NO_2 in our model atmosphere. This was pointed out to us[6] at the conclusion of the current work. Note that the plume is only twenty meters thick and the

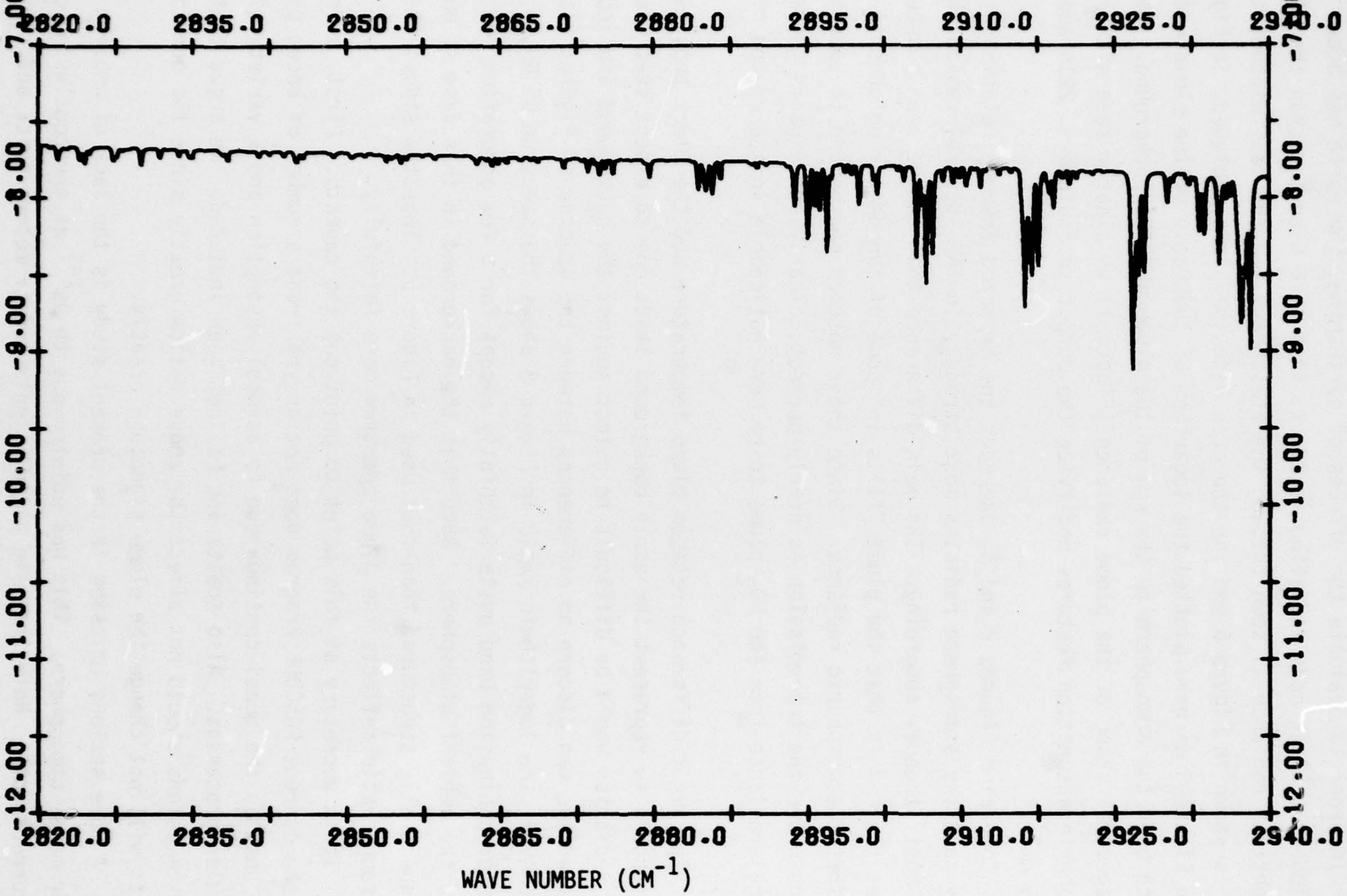

FIGURE 6: Logarithm of the 290 K Earth Background and Atmospheric Spectral Radiance (watts/cm^2/ster/cm^{-1}) Without a Plume.

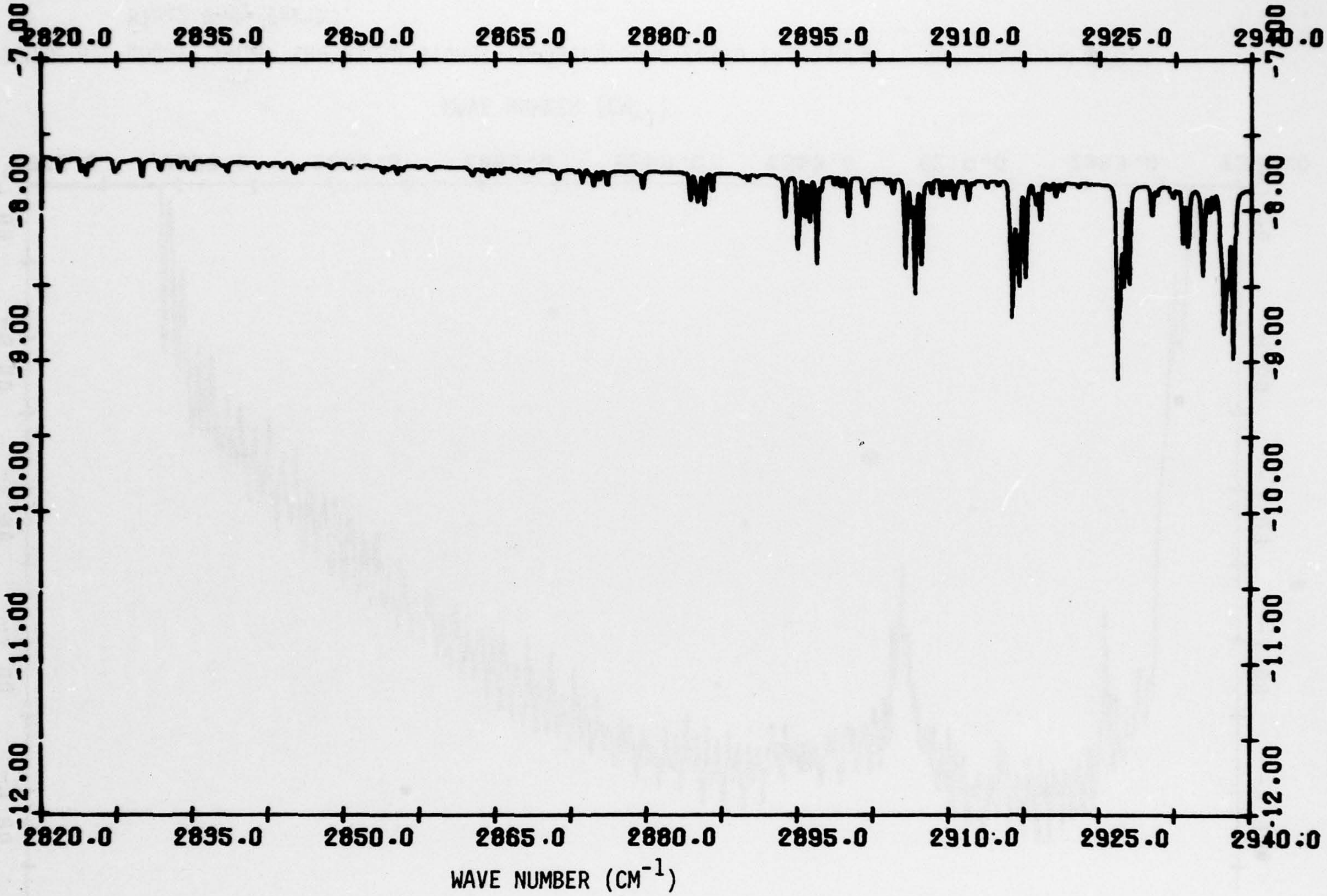

FIGURE 7: Logarithm of the 290 K Earth Background and Atmospheric Spectral Radiance (watts/cm^2/ster/cm^{-1}) With a Plume.

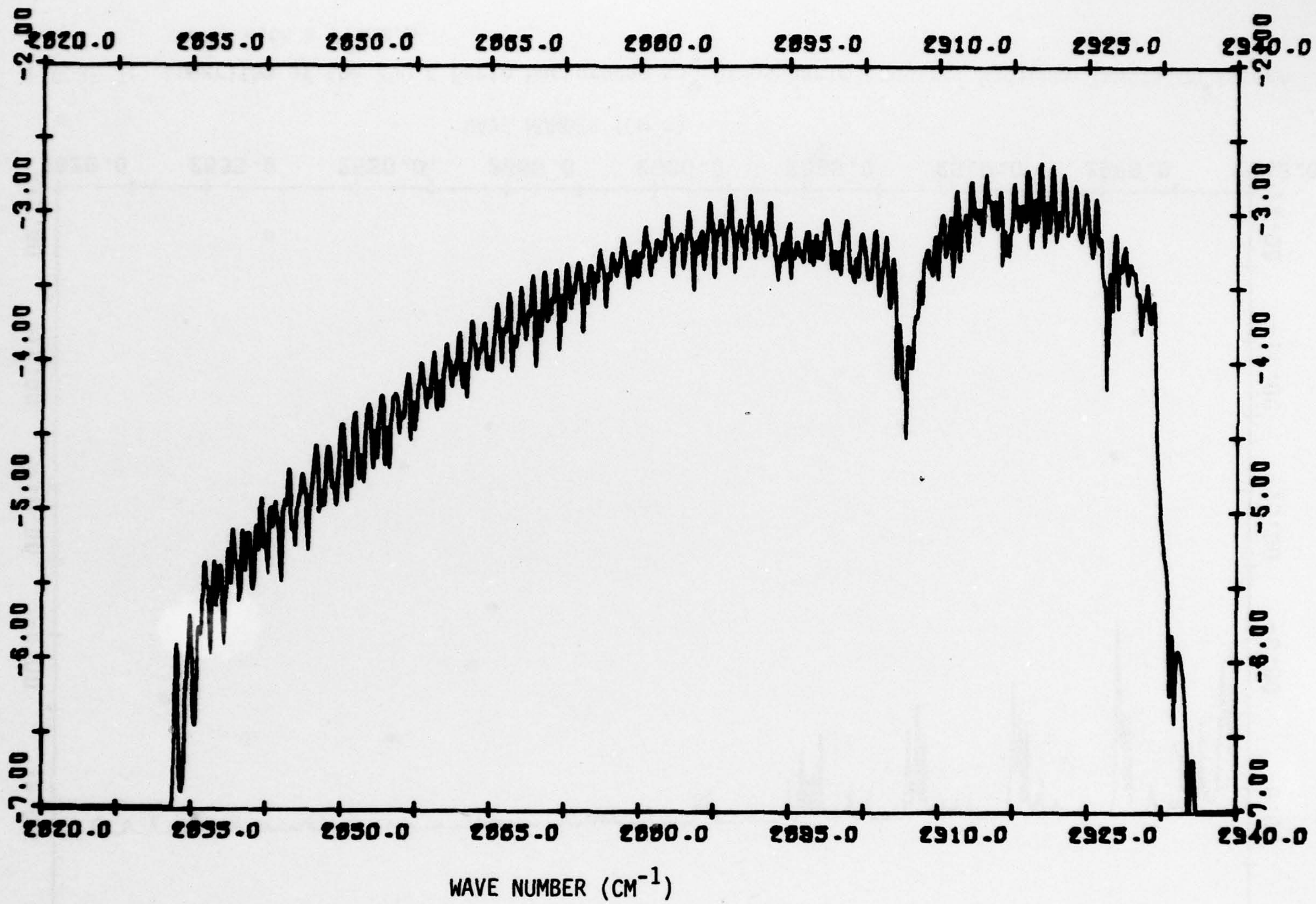

FIGURE 8: Logarithm of the Plume Signal-to-Background Ratio (Atmospheric Radiance and 290 K Black Body Earth).

ambient NO_2 concentration is only 10^{-3} of the plume concentration. Since the total path length is more than twenty kilometers, it is possible that the integrated density of NO_2 along the path to space is comparable to that in the plume. If we assume that the ambient NO_2 concentration is properly represented by a constant mixing ratio η_o and an exponential profile $N_o e^{-h/H}$ we can obtain for the vertical integrated density

$$s = \eta_o N_o \int_0^\infty \exp(-h/H)\, dh = \eta_o N_o H \tag{1}$$

where H is the scale height and N_o is the total number density at the earth's surface. The corresponding quantity for the plume is $s_p = \eta_p N_o d$ where η_p is the plume mixing ratio and d the plume thickness. The ratio of these two is then

$$\alpha \equiv s_p/s = \eta_p d/\eta_o H \tag{2}$$

For $\eta_o = 10^{-9}$, $\eta_p = 10^{-6}$, d = 20 m and H = 6.3 km, α is ~ 3. Thus for constant η_o and a vertical path, the plume should dominate. It must be pointed out however, that there are indications that the ambient profile of NO_2 is far from exponential[2, 7]. If this is so, then it is possible that the NO_2 plume would no longer have a larger integrated absorber amount than the ambient. However, the plume would still be the highest temperature feature. Thus one expects that the higher layers will act primarily as absorbers of the plume radiation with a resulting degradation in the signal-to-noise ratio defined above. The spectral shape would be modified due to narrower absorption line widths in the cooler layers above the plume. Qualitatively then one might expect that our conclusions would hold. However, if the amount of NO_2 in the ambient column is much greater than in the plume, the absorption at the lower temperatures could change the spectral shape appreciably and perhaps decrease the possibility of discriminating the plume.

Finally, it should be pointed out that the question of atmospheric NO_2 be addressed further using FASCODE given a greater effort than we have been able to expend at this time. We also point out the possibility of exploring

NO_2 profiles from spacecraft using solar and stellar extinction techniques. Given sufficient resolution of the spacecraft instrumentation, molecular temperatures could also be inferred. If these inferred temperatures differ significantly from kinetic temperatures as measured or obtained from reliable models, one might hope to obtain data on non-equilibrium processes due to collisions, photo-absorption and chemistry for example, the reaction

$$NO + O_3 \rightarrow NO_2 + O_2 \qquad (3)$$

Such a possibility can be investigated with the aid of FASCODE in conjunction with other computer models.

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